Theoretical investigation on 4*f* electron character of $CeIn_3$ and $CeSn_3$ by means of 3*d*-4*f* inelastic resonant X-ray scattering

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Ce intermetallics, which are typical strong correlation systems, show a variety of unusual and interesting macroscopic properties, e.g., heavy fermion behavior, multipole ordering, Kondo effects, and super conductivity. In order to understand these properties of Ce intermetallics, the character of Ce 4*f* electron is roughly categorized into the dominant regime of the so-called Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction and that of Kondo effect in Doniach phase diagram [1]. In the RKKY regime, Ce 4*f* electron is localized character, and various types of magnetically ordered state are realized, e.g., antiferromagnetic ordering is observed below 10.2 K in $CeIn_3$ [2,3]. On the other hand, in the Kondo regime, Ce 4*f* electron is itinerant character, and valence fluctuation occurs with high Kondo temperature (T_k) which is a characteristic physical quantity for Kondo effects, e.g., T_k is around 200 K in $CeSn_3$. Then, it is well known that the difference of 4*f* character between the RKKY regime and Kondo regime is caused by the difference in the hybridization strength between Ce 4*f* electron and conduction electrons, so-called *c-f* hybridization, thus the investigation of Ce 4*f* electron state is essential to clarify comprehensively the various properties of Ce intermetallics.

In order to study the different electron states of $CeIn_3$ and $CeSn_3$ with the same $AuCu_3$-type crystal structure, we employ an impurity Anderson model considering full multiplet effects in addition to a realistic band effect based on a local density approximation calculation [4]. Moreover, in order to discuss quantitatively the electron state of $CeIn_3$ and $CeSn_3$, we describe the many-particle wave function within a configuration interaction scheme including electron-hole pair excitations [5]. In this study, we performed the calculation of 3*d*-4*f* inelastic resonant X-ray scattering (RIXS), and found that we directly acquire the binding energy of Kondo singlet formation by means of the 3*d*-4*f* RIXS under the depolarized geometry. Moreover, form the 3*d*-4*f* RIXS under the polarized geometry, we can obtain the information of itinerant component of the Kondo singlet [5].

[1] S. Doniach, Physica B & C **91**, 231 (1977).
[2] K. H. J. Buschow, H. W. de Wijin and A. M. van Diepen, J. Chem. Phys. **50**, 137 (1969).
[3] J. M. Lawrence and S. M. Shapiro, Phys. Rev. B **22**, 4379 (1980).
[4] H. Tonai, N. Sasabe, T. Uozumi, N. Kawamura and M. Mizumaki, J. Phys. Soc. Jpn. **86**, 093704 (2017).
[5] N. Sasabe, H. Tonai and T. Uozumi, J. Phys. Soc. Jpn. **86**, 093701 (2017).